

Quasiparticle Scattering Interference in High Temperature Superconductors

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We propose that the energy-dependent spatial modulation of the local density of states seen by Hoffman *et al* [4] is due to the scattering interference of quasiparticles. In this paper we present the general theoretical basis for such an interpretation and lay out the underlying assumptions. As an example, we perform exact T-matrix calculation for the scattering due to a single impurity. The results of this calculation is used to check the assumptions, and demonstrate that quasiparticle scattering interference can indeed produce patterns similar to those observed in Ref. [4].

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Lately the possibility that a competing charge density wave order exists in $Bi_2Sr_2CaCu_2O_{8+\delta}$ has received a lot of attention in scanning tunnelling microscopy (STM) studies. For example, by applying a magnetic field Hoffman *et al* observed a four-lattice-constant modulation of the local density of states (LDOS) along the $(0, \pm 1)$ and $(\pm 1, 0)$ crystalline directions in regions surrounding the cores of superconducting vortices[1]. Quite recently Howald *et al* reported similar LDOS modulation in *zero* magnetic field for a relatively wide range of bias voltage[2]. These results have stimulated considerable interests in the high- T_c community[3]. Recently Hoffman *et al* re-examined the zero-field LDOS modulations using high resolution Fourier-transform-scanning tunnelling-spectroscopy[4]. They found a very important result - the period of the LDOS modulation changes with bias voltage. One of us (DHL) proposed that this phenomenon can be explained in terms of the quasiparticle scattering interferences (QSI).

Scattering interference is an elementary concept in quantum mechanics. In a nut shell, an incoming wave is scattered into outgoing wave by some kind of perturbation; the interference between the two partial waves gives rise to a spatial modulation of the amplitude of the total wave. LDOS modulation due to the scattering interference has been long observed for normal metals[5]. In the context of high- T_c , it has been suggested that the LDOS modulation due to quasiparticle interference bears interesting information on the pairing symmetry of Cooper pairs[6].

The purpose of the present paper is to lay down the theoretical basis for the QSI interpretation of Hoffman *et al*'s data. In particular we spell out the key assumption which allows the deduction of the normal state Fermi surface and the superconducting gap dispersion from the observed LDOS modulations[4, 7]. As a sanity check, we perform exact (numerical) scattering calculation for the case of a single impurity. The results are used to demonstrate the validity of our assumption and that QSI can indeed produce LDOS modulation patterns similar to those observed by STM.

Now we briefly summarize the findings of Ref.[4]. By examining the magnitude of the Fourier transformed LDOS Hoffman *et al* found two discernible groups of modulation wave vectors. The first is in the $(0, \pm 1)$ and $(\pm 1, 0)$ directions and the second is in the $(\pm 1, \pm 1)$ directions. The wave vectors \mathbf{q} of the first/second group disperse with bias voltage V in such a way that $|\mathbf{q}|$ decreases/increases when $|V|$ increases. In addition, for fixed V , the $|\mathbf{q}|$ in the first/second group decreases/increases with doping. In Ref.[4] this two group of wavevectors are identified as the momentum transfer when a quasiparticle is elastically scattered across the normal state Fermi surface as indicated by the numbered arrows 1 and 2 in Fig.1. Based on this interpretation Hoffman *et al* were able to deduce the Fermi surface location and superconducting gap function, and found fairly good agreement with the results of angle-resolved photoemission experiment[8].

Formally the idea used in Ref.[4, 7] can be precisely stated in the following Greens function formalism. Let $G_0(\mathbf{k}, \omega)$ be the (2×2) single-particle Greens function in the superconducting state in the absence of scattering, and $T(\mathbf{k} + \mathbf{q}, \mathbf{k}; \omega)$ be the 2×2 scattering matrix for the $\mathbf{k} \rightarrow \mathbf{k} + \mathbf{q}$ transition. The Fourier transform of the local density of states is given by

$$\begin{aligned} n(\mathbf{q}, \omega) &= n_0(\mathbf{q}, \omega) - \frac{1}{2\pi i} [A_{11}(\mathbf{q}, \omega) + A_{22}(\mathbf{q}, -\omega) \\ &\quad - A_{11}^*(-\mathbf{q}, \omega) - A_{22}^*(-\mathbf{q}, -\omega)] \\ A(\mathbf{q}, \omega) &= \int \frac{d^2 k}{(2\pi)^2} G_0(\mathbf{k} + \mathbf{q}, \omega) T(\mathbf{k} + \mathbf{q}, \mathbf{k}; \omega) G_0(\mathbf{k}, \omega). \end{aligned} \quad (1)$$

In the above the subscript "0" implies the absence of scattering. Given Eq. (1) if one makes the assumption (the "on-shell" assumption) that the integral in $A(\mathbf{q}, \omega)$ is dominated by those \mathbf{k} 's that satisfy the simultaneous pole equations for both G_0 's, one obtains the result needed for the QSI interpretation of Ref.[4, 7]. In particular one concludes that at a given bias $eV = \omega$, $|n(\mathbf{q}, \omega)|$ is the largest when there is a large joint density of states

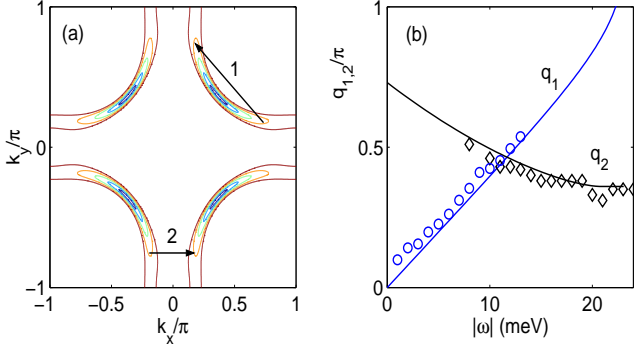


FIG. 1: (a) Schematic plot of banana-shaped equal-energy contours. Contours at higher energies are not shown. The tips of the bananas traces the normal state Fermi surface. The arrows indicate important elastic scattering processes discussed in the text. (b) The energy dependence of the modulation wave vector $q_{1,2}$ associated with the scattering processes 1 and 2 indicated in (a). The solid lines are naive expectations, and the symbols are extracted from such pictures as plot in Fig.2. A symbol is put down for a particular energy only when there is a discernable peak in the wave vector space. It is interesting to note that only in a narrow energy range peaks in both direction coexist.

associated with scattering wavevector \mathbf{q} .

The normal state Fermi surface of Bi-2212 consists of four hole-like segments.[9] To get a feel of the joint density of states let us first concentrate on the curves of constant energy (CCE) for the quasiparticles. (Since experimentally LDOS modulation is only observed for energies lower than ~ 30 meV, we shall concentrate on that energy range here.) Around each of the four gap nodes the CCE evolves from a single point at zero energy, to banana-shaped closed contours at higher energies. The size of the banana increases with the energy until its tips touch the Brillouin zone. When that happen the CCE changes from closed to open contours. This is schematically shown in Fig.1, where different CCE's represent different quasiparticle energies. Due to the large difference between v_F and v_Δ ($v_F/v_\Delta \approx 20$ at the gap nodes, v_F = the normal state Fermi velocity, and v_Δ = the derivative of the superconducting gap along the direction tangential to the Fermi surface) the CCE moves with energy the fastest at the tips of the banana. As a result we expect those \mathbf{q} 's connecting the tips to have the largest joint density of states. This argument leads to the prediction that the most prominent LDOS modulation wave vectors should be the set of vectors connecting pairs of banana tips[7].

As we pointed out earlier, the above expectations are based on the on-shell approximation. The result of an exact scattering calculation using Eq. (1) can in principle deviate from the above expectations due to the following complications. 1) The “off-shell” contributions: i.e. those \mathbf{k} 's that do not fulfill the simultaneous pole equations of the two G_0 's in Eq. (1). These off-shell contribu-

tions act to blur the modulation wave vectors predicted above. 2) The effects of scattering matrix element. Even when the on-shell approximation works well, the intensity of the actual LDOS modulation can depend on the actual scattering matrix element, which in turn depends on the coherence factor. For example when the scattering is due to a single scalar (V_s) and/or magnetic (V_m) impurity, the $\mathbf{k} \rightarrow \mathbf{k}'$ scattering matrix element is proportional to $(V_m + V_s)u_k u_{k'} + (V_m - V_s)v_k v_{k'}$, with $u_k = \pm \text{sgn}(\Delta_k) \sqrt{(1 \pm \epsilon_k/E_k)/2}$, $v_k = \sqrt{(1 \mp \epsilon_k/E_k)/2}$. In the above the upper/lower sign applies for positive/negative energy quasiparticle states, ϵ_k is the normal state dispersion, Δ_k is the gap function, and $E_k = \sqrt{\epsilon_k^2 + \Delta_k^2}$. For d-wave pairing Δ_k changes sign in some of the scattering processes and not in others. For example in Fig.1 Δ_k changes sign in the process labelled by the numbered arrow 1, while maintains the same sign in the process labelled by the numbered arrow 2. Therefore depending on whether the scattering process is caused by scalar or magnetic impurity processes 2 or 1 will be relatively suppressed.

In the following we perform an exact calculation where the scattering is caused by a single impurity. The purpose of this calculation are two folds: 1) through an exact calculation we can check the on shell assumption that is crucial to interpretation of Hoffman *et al*'s data. 2) Through the exact calculation we can find out whether the effect of scattering matrix element can make the scattering interference patterns different from those expected from the joint density of state argument. This type of calculation (i.e. an impurity in an d-wave superconductor) is certainly not new[11]. However as far as we know it is the first that demonstrate QSI can indeed give rise to LDOS modulation patterns observed by STM[4, 7]. Here is the summary of our results: 1) we find that among the possible wavevectors the most pronounced LDOS modulation are associated scattering processes 1 and 2 (and their symmetry equivalence) in Fig. 1. The Fourier transforms of the LDOS are given in Fig.2. A comparison between the $\mathbf{q} - \omega$ dispersion expected from the joint density of states argument and that extracted from Fourier transforming the exact LDOS modulation is given in Fig.1(b).

For the quasiparticle Hamiltonian, we use a model provided by Norman *et al*[10]:

$$H = \sum_{k\sigma} \epsilon_k C_{k\sigma}^\dagger C_{k\sigma} - \sum_k (\Delta_k C_{k\uparrow} C_{-k\downarrow} + \text{h.c.}). \quad (2)$$

In the above $\epsilon_k = \sum_{n=0}^5 t_n \chi_n(k)$ and $\Delta_k = \Delta_0 (\cos k_x - \cos k_y)/2$, where $t_{0-5} = 0.1305, -0.5951, 0.1636, -0.0519, -0.1117, 0.0510$ (eV), and $\Delta_0 = 0.025$ eV. Moreover $\chi_{0-5}(k) = 1, (\cos k_x + \cos k_y)/2, \cos k_x \cos k_y, (\cos 2k_x + \cos 2k_y)/2, (\cos 2k_x \cos k_y + \cos 2k_y \cos k_x)/2$, and $\cos 2k_x \cos 2k_y$. The $G_0(\mathbf{k}, \omega)$ and $T(\mathbf{k} + \mathbf{q}, \mathbf{k}; \omega) [= T(\omega)$ for a single impurity] in Eq.(1) are given by,

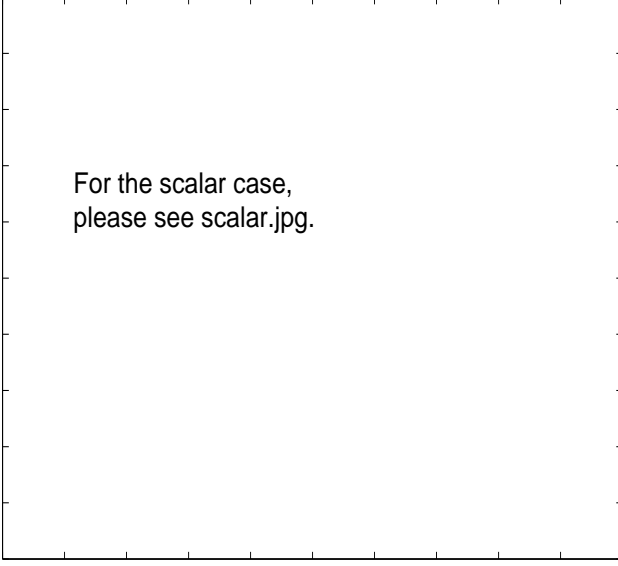


FIG. 2: Fourier amplitudes of the LDOS maps at the given energies as a function of momenta in the first Brillouin zone for $(V_s, V_m) = (100\text{meV}, 0)$. The numbers on the sub-graphs show the energy in units of meV. The hot/cold color denotes higher/lower strength.

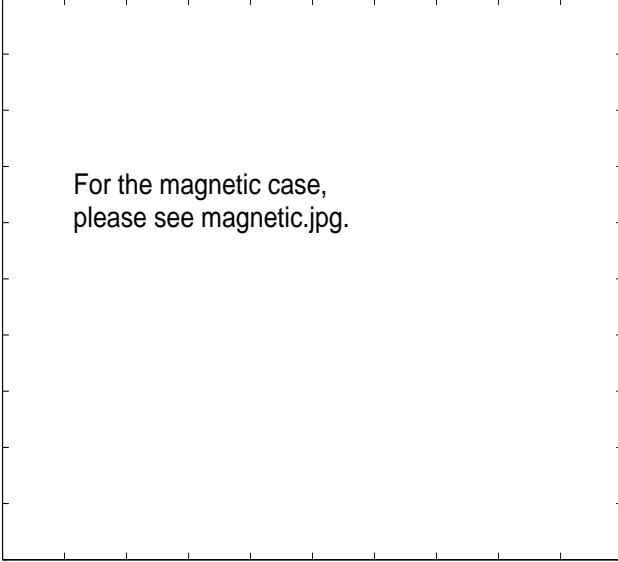


FIG. 3: The same as Fig.2 for $(V_s, V_m) = (0, 100\text{meV})$.

respectively,

$$G_0^{-1}(\mathbf{k}, \omega) = (\omega + i\delta)I - \epsilon_{\mathbf{k}}\sigma_3 - \Delta_{\mathbf{k}}\sigma_1$$

$$T^{-1}(\omega) = (V_s\sigma_3 + V_m I)^{-1} - \int \frac{d^2k}{(2\pi)^2} G_0(\mathbf{k}, \omega), \quad (3)$$

where σ_i 's are the Pauli matrices.

In order to accurately take into account the contribu-

tion to G_0 from the thin bananas in Fig.1(a), a momentum resolution $\delta k \ll \pi v_{\Delta}/v_F$ must be achieved. This in turn means that a large real space lattice has to be used for the actual calculation. For the results reported below a 400×400 lattice is used. In this calculation we did not take the self-consistent suppression of the pairing amplitude near the impurity into account. However we do not expect this omission to cause any significant change because the impurity scattering strength we used is much larger than the maximal pairing gap.[12]

In the following two kinds of impurities are studied: (a) non-magnetic impurity ($V_s = 100\text{meV}$ and $V_m = 0$) and (b) magnetic impurity ($V_s = 0$ and $V_m = 100\text{meV}$). By using two extreme types of scatterer we can study the effect of matrix element on the QSI pattern. The impurity strength we choose is intermediate in the sense that we do not see quasiparticle resonance states in the LDOS.[13] It is interesting that although this type of impurity does not show up in the zero bias resonance image, they do have important effect on the LDOS modulation.

Fig.2 shows the Fourier amplitude of the LDOS maps at $\omega = -24 \rightarrow -3$ meV and $\omega = 3 \rightarrow 24$ meV with 3 meV interval for a nonmagnetic. In these figures the intensity at $\mathbf{q} = 0$ is subtracted so that weaker features at other wave vectors can show up. In constructing Figure 2 the LDOS of the central 51×51 plaquette in the 400×400 lattice are Fourier transformed. It is interesting to note that in real experiment a large field of view is also employed in the Fourier transform in order to achieve high momentum resolution.

For the negative energies in Fig.2 the Fourier peaks in the $(\pm 1, \pm 1)$ direction is clearly visible between -3 to -12 meV. Moreover as the binding energy increases the peaks moves away from the origin. For binding energy 18 meV and above the Fourier peaks in the $(0, \pm 1)$ and $(\pm 1, 0)$ appear. Contrary to the diagonal direction spots these peaks move only slightly as the energy varies. Careful analysis of such movement indicates that these peaks move toward the origin as the binding energy increases. The energy dependence of the these LDOS Fourier peaks is shown in Figure 1(b) as symbols. The difference between the naive expectation (solid lines) and the results of T-matrix calculation (symbols) is very small. This comparison clarifies the extent by which the qualitative picture of joint density of states works. In addition to the above peaks there are other weaker features in Fig.2. These features can either be identified as the higher harmonics of the diagonal and vertical/horizontal spots or can be attributed to the other scattering processes not shown in Fig.1[7]. Upon the reversal of the bias voltage we find the diagonal Fourier peaks become much weaker. On the contrary the $(0, \pm 1)$ and $(\pm 1, 0)$ direction peaks seem to be insensitive to the bias reversal[14].

The quasiparticle interference patterns for magnetic impurity in Fig.3 are quite different from those shown in Fig.2. For example the amplitude of the $(\pm 1, \pm 1)$ direction modulation for $|\omega| \leq 12$ meV is much weaker. The fact that the $(\pm 1, \pm 1)$ direction peaks are weaker

than the $(\pm 1, 0)$ and $(0, \pm 1)$ direction peaks is consistent with the coherence factor effect discussed previously.

In addition to the above differences there are similarities between Figs. 2 and 3. For example at $|\omega| = 21, 24$ meV, the patterns in these figures become rather similar. In the same energy range the asymmetry between positive and negative bias becomes small. In this energy range the horizontal component of the scattering wavevector associated with process 2 cease to change with energy. As the result the modulation wave-vectors in the $(\pm 1, 0)$ and $(0, \pm 1)$ directions hardly change.

Upon closing a few remarks are in order. 1) The present result demonstrates that QSI due to scattering by scalar (non-unitary) impurities can produce LDOS modulation similar to that observed in recent STM experiment[4, 7]. This effect is due to quantum interference, and does not require the presence of a charge density wave order. 2) Whether the phenomenology of a very weak/fluctuating charge density wave order is consistent with the experimental observations[4, 7] should be further investigated[2, 15]. 3) The results of the present paper is obtained assuming sharply defined quasiparticles in the superconducting state[16]. However our general formulation (Eq. (1)) allows us to treat not so well defined quasiparticles as well - all we have to do is to

modify the sharp pole structure of G_0 . We find that the $(\pm 1, 0)$, $(0, \pm 1)$ direction modulation is robust against quasiparticle life time broadening whereas the $(\pm 1, \pm 1)$ direction modulation is not. 4) In the present paper we use a single impurity as a representative of elastic quasiparticle scatterer. However we believe that the QSI idea should work under wider circumstances. 5) It is not clear to us what is the main source of quasiparticle scattering in BSCCO. For example, recently Podolsky *et al* argued that scattering by a disordered charge density wave could give rise to similar energy dependent $(\pm 1, 0)$ or $(0, \pm 1)$ modulations as well[17]. 6) Finally, what is the relation between the relatively weak quasiparticle interference observed at zero magnetic field[4, 7] and the relatively strong checkerboard LDOS modulation near superconducting vortices[1] is currently unclear.

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- [1] J. Hoffman, *et al*, Science **295**, 466 (2002).
 - [2] C. Howald, H. Eisaki, N. Kaneko, and A. Kapitulnik, cond-mat/0201546.
 - [3] See, *e.g.*, S. Sachdev, cond-mat/0203363 (and references cited therein); M. Vojta, cond-mat/0204284; Han-Dong Chen, *et al*, cond-mat/0203332; Jian-Xin Zhu, Ivar Martin, and A. R. Bishop, cond-mat/0201519; M. Franz, D. E. Sheehy, and Z. Tesanovic, cond-mat/0203219.
 - [4] J. Hoffman *et al*, to appear in Science.
 - [5] M.F. Crommie *et al*, Nature **363**, 524 (1993).
 - [6] J.M. Byers, M.E. Flatte and D.J. Scalapino, Phys. Rev. Lett. **71**, 3363 (1993); M.E. Flatte, and J.M. Byers, Phys. Rev. Lett. **80**, 4546 (1998).
 - [7] K. McElroy *et al* submitted to Nature.
 - [8] H. Ding *et al*, Phys. Rev. B **54**, R9678 (1996).
 - [9] For a review of the angle-resolved-photo-emission study of the electronic structure in the cuprates, see, *e.g.*, A. Damascelli, D.H. Lu, Z.-X. Shen, J. Electron Spectr. Relat. Phenom. **117-118**, 165 (2001) (cond-mat/0107042), and references cited therein.
 - [10] M. R. Norman, M. Randeria, H. Ding and J. C. Cam-puzano, Phys. Rev. B **52**, 615 (1994).
 - [11] LDOS modulation caused by impurities has been studied by *e.g.* M Choi, Phys. Rev. B **50**, 3491 (1994); T. Xiang and J.M. Wheatley, Phys. Rev. B **51**, 11721 (1995).
 - [12] In the presence of order parameter suppression there is an additional anomalous scattering potential (due to the change in the gap parameter) around the location of the impurity. However the strength of this anomalous scattering potential is bounded above by the maximal pairing gap in the bulk. Since the scalar potential is much stronger its effects dominate. We have done extensive calculations where there are both scalar and anomalous scattering potentials. The above statement has been checked carefully.
 - [13] See, *e.g.*, A. V. Balatsky, M. I. Salkola, and A. Rosengren, Phys. Rev. B **51**, 15547 (1995); M. I. Salkola, A. V. Balatsky, and D. J. Scalapino, Phys. Rev. Lett. **77**, 1841 (1996); Qiang-Hua Wang, Phys. Rev. Lett. **88**, 057002 (2002); H. Tsuchiura, Y. Tanaka, M. Ogata, S. Kashiwaya, Phys. Rev. Lett. **84**, 3165 (2000).
 - [14] We have investigated the asymmetry of the $(\pm 1, \pm 1)$ direction Fourier peaks upon bias reversal further. We find such asymmetry depends on the detailed quasiparticle dispersion. For example by setting all the t_n except $n = 1$ to zero we find the asymmetry disappears. Thus we conclude that we have investigated the issue of plus/minus bias voltage asymmetry of the $(\pm 1, \pm 1)$ direction Fourier peaks further. We find the detailed quasiparticle dispersion has important effects on this asymmetry. For example by setting all the t_n except $n = 1$ to zero we find the asymmetry disappears. Therefore we conclude that we can not make a definitive prediction of the bias asymmetry.
 - [15] S.A. Kivelson private communication.
 - [16] For the cuprates the quasiparticles are poorly defined above T_c . Below T_c they become better-defined; D. L. Feng, *et al*, Science **289**, 277 (2000); H. Y. Kee, C. M. Varma, Phys. Rev. B **58**, 15035 (1998).
 - [17] D. Podolsky, E. Demler, K. Damle, and B.I. Halperin, cond-mat/0204011.

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